Taming and Accelerating Particle-In-Cell

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Particle-In-Cell (PIC) codes are among the most widely used simulation methods today, essential components of the state-of-the-art in fluid dynamics, plasma and beam physics, and astrophysics and cosmology. Major applications include solid state device design, accelerator physics, galaxy formation, fusion reactors, fluid flows, and magnetohydrodynamics (MHD). Typically, leading-edge PIC simulations are large parallel codes, the number of simulation particles running into the billions, fully 3D (with or without sub-grid modules), and possessing spatial dynamic range anywhere between two to five orders of magnitude. Since particle codes are—by their very nature—extremely memory and computation-intensive, it is not surprising that much effort has been expended over the years in addressing these two issues. As a result, the codes now have sufficient statistical power and dynamic range so that, in several important applications, quantitative assessments of code robustness and accuracy are possible in principle and in fact will soon become absolutely necessary. In other words, these PIC applications are now at a threshold where they can be used for precision prediction rather than just as quantitative indicators of system behavior. However, before this threshold can be crossed, error control and code verification must be sharpened to an entirely new level; attaining this level is the aim of our project.

While we are targeting general issues of error control and performance acceleration, it is also important to focus on specific application test-beds. In our work, these are accelerator physics (beam dynamics) and astrophysics and cosmology (galaxy distribution and formation). Particle accelerators are among the largest, most complex, and most important scientific instruments in the world. The design of the next generation of accelerators requires a new level of simulation capability as designers push the boundaries of beam intensity, energy, and system complexity. Particle simulation lies at the heart of treating the gravitational interaction in astrophysics and cosmology, the engine underlying the largest and the most energetic phenomena in the universe. Several recent observations and planning for next-generation ground-based and space missions require PIC and hybrid simulations of a scale and precision that have yet to be approached. Successful acceleration and verification of PIC codes in these challenging applications will not only be intrinsically important but signal the viability of these methods to other simulation arenas.

The fundamental reason why PIC codes are not straightforward to analyze is because they are not partial differential equation (PDE) solvers. Even though the underlying equation for the particle distribution function (PDF) satisfies a PDE (e.g., Vlasov-Poisson or Vlasov-Maxwell), the particle sampling of a smooth distribution introduces an intrinsic discreteness in the numerical description. In addition, an important reason for employing particle codes is that they are insensitive to the generation of arbitrarily fine scales in the evolution of the PDF, which would cause a direct PDE solver to either stall or crash. Thus, the correct way to view a PIC simulation is as a statistical dynamical Monte Carlo evolution; essentially a method to generate statistical information as sampled by the particles, the individual trajectories being of no intrinsic importance. The statistical information is encoded in moments of the PDF, hence, the central issue relates to the evolution of these moments and how well they can be characterized by a finite number of tracer particles. While the individual particle trajectories can be chaotic, we have shown that the exact moment equations are regular for a wide class of systems. This is the starting existence result for a true statistical theory of PIC errors.

In a PIC simulation, an initial PDF is sampled by particles, the particle distribution is mapped to a discrete charge or density field on a grid, the Poisson equation is solved on the grid, the gradient of the potential (i.e., the self-consistent force) interpolated back on to the simulation particles, and a forward time-step taken using this force. The procedure is then repeated as many times as desired. While apparently disarmingly simple, the process is actually far from that. Several questions can be immediately noted: How accurately can the PDF and its moments be sampled by a finite number of particles? How does the associated "discreteness noise" propagate in the evolution? How does the finite dynamic range of a simulation affect the formation of structure and substructure in the particle simulation? What are the numerical effects of short- and long-range particle collisions on what is supposedly a collisionless simulation? And so on.

Once the convergence of certain quantities is established and understood, powerful extrapolation methods can be used to improve code performance. For example, we have shown that Richardson extrapolation can be used to improve the convergence of the particle velocity distribution as well as the power spectrum in cosmology simulations. Additionally, we have developed a methodology for estimating the effects of collisionality in N-body simulations. However, as shown in the figures, more complex topological questions such as the errors associated with generation of substructure as code force resolution is increased remain to be understood.

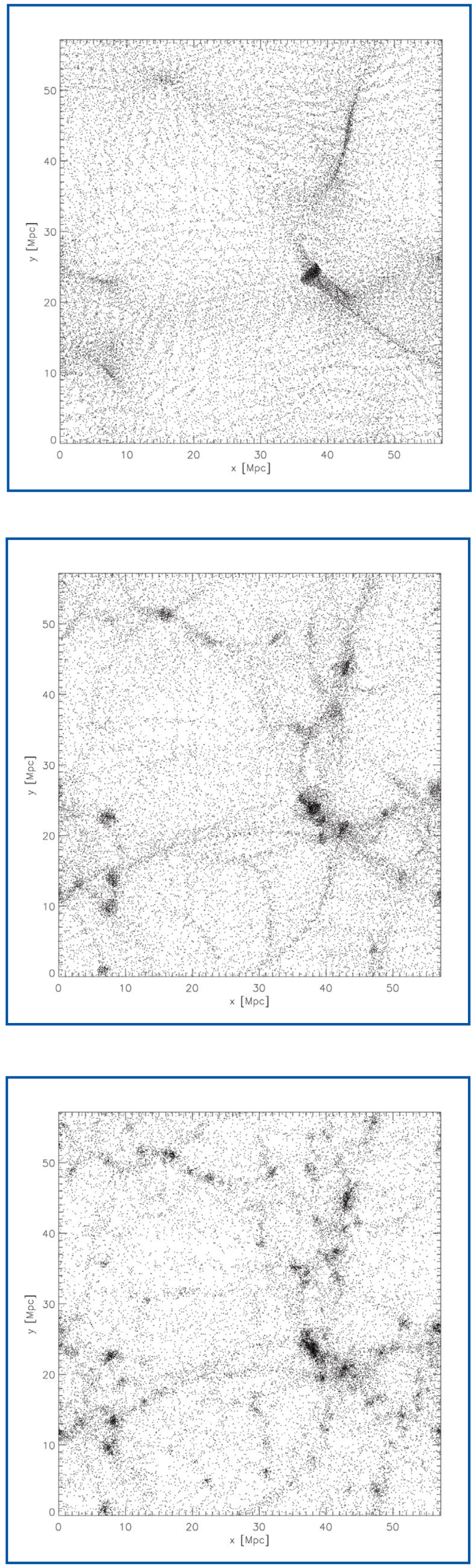

Figure 1—
The effect of resolution in the formation of structure in a 3D cosmology code. In the three figures, the particle initial conditions were identical, however the force resolution was increased by successive powers of two. Note that the single "knot" and filamentary structures of the first figure have broken up into finer filaments and substructures as the resolution is increased. At present, error-control methodologies are incapable of treating this situation.